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THE GROUND STATE OF MEDIUM-HEAVY NUCLEI WITH NON CENTRAL FORCES

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1. INTRODUCTION

Correlated Basis Function (CBF) theory is a powerful tool to investigate the properties of many-body strongly interacting systems in several fields of physics. Its first succesful applications are found in homogeneous systems such as liquid Helium, electron systems (both in the forms of electron fluids and lattice structures) and infinite nuclear and neutron matter. The flexibility of CBF based approaches results in a realistic description of ground state (energy, momentum distribution, distribution functions and so on) as well as of dynamical (cross sections) quantities. While the g.s. is often better studied by MonteCarlo (MC) methods, CBF and perturbative theories in a CBF basis still provide one of the very few viable ways for an affordable, quantitative study of the response of many-body systems to external probes. In addition , the nuclear interaction and the induced nucleon-nucleon correlations are strongly dependent on the states of the nucleons themselves, and the MC techniques adopted, for instance, in the case of liquid Helium g.s. are not easily extended to nuclear cases.

As most of the world we know is not homogeneous, CBF addicted began in the last decade to extend the theory (and the connected technologies) to such interesting objects as Helium films and droplets and finite nuclear systems (usually named *nuclei*). In Helium the interaction is known and has a relatively simple form, so the difficulty lies in the large densities. On the contrary, nuclei are considerably less dense and the actual problem is the aforementioned complicated structure of the interaction. Presently, there is a number of methods that exactly solve the light nuclei Schrödinger equation for realistic hamiltonians. Faddeev [1,2], Green Function Monte Carlo (GFMC) [3] and Correlated Hyperspherical Harmonics Expansion [4] are used for the A=3,4 nuclei, and GFMC has been recently pushed up to A=7 [5]. Variational MonteCarlo (VMC) [6] methods has been also used in light nuclei and,

if the spanned variational wave function space is large enough, then its description may be quite accurate (even if not exact). VMC has been extended to heavier nuclei, as ^{16}O [7].

As the mass number, A, grows larger and the region of medium-heavy nuclei is approached, using MC with realistic hamiltonians becomes increasingly difficult and CBF theory and cluster expansions represent an alternative and a competitive approach. In a series of papers, doubly closed shell nuclei (both in *ls* and *jj* coupling) were studied using the Fermi hypernetted chain (FHNC) [8] summation technique [9,10,11]. Semirealistic, central interactions and simple two-body correlations, depending on the interparticle distances and, at most, on the isospin of the correlated pair, were used and nuclei ranging from ^{4}He to ^{208}Pb were investigated. In a recent paper the same method has been extended to interactions and correlations containing spin, isospin and tensor components for ^{16}O and ^{40}Ca nuclei, having doubly closed shells in *ls* coupling [12]. The review of the results obtained in this work will be the object of the present contribution.

We consider a standard nuclear hamiltonian

$$H = -\frac{\hbar^2}{2\,m}\sum_i \nabla_i^2 + \sum_{i<j} v_{ij} \quad , \tag{1}$$

containing only a two-nucleon potential, v_{ij}, whose large interparticle distances behavior is dominated by meson exchange processes (one pion exchange, OPE). The intermediate and short distances parts of the potential are generally treated in semimicroscopic or purely phenomenological ways and several recipies are on the market. Their common feature is the accurate fit to the large body of available two nucleon scattering data up to energy ~ 350 MeV. For our purposes, we shall use a truncated version of the realistic Urbana v_{14} model (U14) [13]. U14 is pametrized as the sum of 14 components,

$$v_{14,ij} = \sum_{p=1,14} v^p(r_{ij}) O^p_{ij} \quad , \tag{2}$$

with

$$O^{p=1,6}_{ij} = [1, \sigma_i \cdot \sigma_j, S_{ij}] \otimes [1, \tau_i \cdot \tau_j] \quad , \tag{3}$$

S_{ij} is the tensor operator and the remaining $p > 6$ components contain linear and quadratic spin-orbit ($\mathbf{L} \cdot \mathbf{S}$) and L^2 terms. The $p > 6$ components are not retained in the v_6 (U6) truncation.

A CBF g.s. correlated A-nucleon wave function can be written as

$$\Psi(1, 2...A) = [\mathcal{S} \prod_{i<j} F_{i,j}] \Phi(1, 2...A) \quad , \tag{4}$$

i.e. a symmetrized product of two-body correlation operators, F_{ij}, acting on a mean field state, $\Phi(1, 2...A)$, given by a shell model wave function built up with $\phi_\alpha(i)$ single particle wave functions. F_{ij} is chosen of a form consistent with the interaction,

$$F_{ij} = \sum_{p=1,6} f^p(r_{ij}) O^p_{ij} \quad . \tag{5}$$

The correlation functions $f^p(r)$ are variational since they contain a set of parameters fixed by minimizing the g.s. expectation value of the hamiltonian, $\langle H\rangle = \langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$. $\langle H\rangle$ is expanded in Mayer-like cluster diagrams and infinite classes of these diagrams are summed by FHNC integral equations. The cluster expansion method has been widely applied to both finite and infinite, interacting systems with state independent (Jastrow) correlations .

For a realistic approach to nuclear systems, the correlation operators are strongly state dependent and do not commute between each other. This fact prevents from the development of a complete FHNC theory for the correlated wave function of eq.(4). A single operator chain (SOC) approximation was adopted in ref.[14] for the operatorial ($p > 1$) correlations, together with a a full FHNC treatment of the Jastrow ($p = 1$) part in nuclear matter (NM). FHNC/SOC apparently provides a satisfying description of infinite nuclear matter at saturation density and a neutron matter equation of state compatible with the neutron stars observational data [15]. However, no exact check for FHNC/SOC is presently available in infinite nucleon matter, apart the evaluation of some additional classes of diagrams. The estimated accuracy in the g.s. energy has been set to less than 1 MeV at saturation [16,15].

We shall use FHNC/SOC theory to study the g.s. of ^{16}O and ^{40}Ca with the U6 interaction and the ^{16}O results will be compared with cluster MC (CMC) results. In the CMC method the Jastrow contribution is exactly treated by MC sampling, and that from the operatorial components is approximated by considering (via MC) up to four-body cluster terms. Higher order contributions are then extrapolated.

2. ONE- AND TWO-BODY DENSITIES AND THE EXPECTATION VALUE OF THE HAMILTONIAN

The one- and two-body densities, $\rho_1(\mathbf{r}_1)$ (OBD) and $\rho_2^p(\mathbf{r}_1,\mathbf{r}_2)$ (TBD), enter (more or less explicitely) the evaluation of $\langle H\rangle$. They are defined as

$$\rho_1(\mathbf{r}_1) = \langle\sum_i \delta(\mathbf{r}_1 - \mathbf{r}_i)\rangle \quad , \tag{6}$$

and

$$\rho_2^p(\mathbf{r}_1,\mathbf{r}_2) = \langle\sum_{i\neq j} \delta(\mathbf{r}_1 - \mathbf{r}_i)\delta(\mathbf{r}_2 - \mathbf{r}_j)O_{ij}^p\rangle \quad . \tag{7}$$

The FHNC theory for the TBD in presence of Jastrow correlations is described at length in ref.[9] and here it is given as granted. Let's just recall that it is written in terms of the Jastrow correlation, $f^J(r) = f^1(r)$, and of the *nodal* (or *chain*) and *elementary* (or *bridge*) functions, $N_{xy}(\mathbf{r}_1,\mathbf{r}_2)$ and $E_{xy}(\mathbf{r}_1,\mathbf{r}_2)$, representing the sums of the diagrams having those topological structures, respectively. The (xy) classification corresponds to the exchange character of the external points (1,2): $x(y) = d, e$ with d =direct (the point does not belong to any exchange loop), e =exchange (the point does belong to a closed exchange loop). Futhermore, $(xy = cc)$ (c =cyclic) diagrams are present, whose external points both belong to the same, non closed exchange loop.

In presence of operatorial correlations, the nodal functions acquire a state dependence, $N^p_{xy}(\mathbf{r}_1,\mathbf{r}_2)$. Because of the non commutativity of the correlations, the same topological diagrams may originate from several different orderings. Spin-isospin traces provide a weight to each of the diagrams, which, in turn, depends on the ordering itself. Keeping track of them is not feasible by FHNC-like integral equations and only selected classes of diagrams may be correctly summed. The SOC approximation consists in summing $p > 1$ chains, where each link may contain just one operatorial element and Jastrow dressings at all orders. We remind that operatorial dependence comes also in account of the exchange of two nucleons, as the exchange operator is $P^{ex}_{ij} = -[1 + O^2_{ij} + O^4_{ij} + O^5_{ij}]/4$.

The FHNC/SOC equations are given in ref.[12], where they are solved in the FHNC/0 approximation (corresponding to set to zero the elementary diagrams). The validity of this seemingly crude approximation will be discussed later.

The structure of the OBD is

$$\rho_1(\mathbf{r}_1) = \rho^J_1(\mathbf{r}_1)\left[1 + U^{op}_d(\mathbf{r}_1)\right] + U^{op}_e(\mathbf{r}_1)C_d(\mathbf{r}_1) \quad , \tag{8}$$

with

$$\rho^J_1(\mathbf{r}_1) = \left[\rho_0(\mathbf{r}_1) + U^J_e(\mathbf{r}_1)\right] C_d(\mathbf{r}_1) \quad . \tag{9}$$

$\rho_0(\mathbf{r}_1) = \sum_\alpha |\phi_\alpha(1)|^2$ is the mean field density, $C_d(\mathbf{r}_1) = \exp\left\{U^J_d(\mathbf{r}_1)\right\}$, $U^J_{d(e)}(\mathbf{r}_1)$ are Jastrow vertex corrections and $U^{op}_{d(e)}(\mathbf{r}_1)$ represent operatorial vertex corrections, linked, by integral equations given in refs.[9,12], to the FHNC nodal functions.

A measure of the accuracy of the computed OBD is the degree of fulfilment of its normalization, $S_1 = A$, where

$$S_1 = \int d^3r_1 \rho_1(\mathbf{r}_1) \quad . \tag{10}$$

In addition, the exact TBD has to comply with the pair saturation, $S_2 = 1$, and (for the nuclei we are considering) the isospin saturation, $S_\tau = -1$, properties, with

$$S_2 = \frac{1}{A(A-1)} \int d^3r_1 \int d^3r_2 \rho^{p=1}_2(\mathbf{r}_1,\mathbf{r}_2) \quad , \tag{11}$$

and

$$S_\tau = \frac{1}{3A} \int d^3r_1 \int d^3r_2 \rho^{p=4}_2(\mathbf{r}_1,\mathbf{r}_2) \quad . \tag{12}$$

A spin saturation sum rule, $S_\sigma = -1$, holds only in absence of tensor correlations.

Deviations of the sum rules from their exact values are due to (*i*) the FHNC/0 scheme and (*ii*) the SOC approximation. In ref.[9] was found that E^{ex}_{ee}, *i.e.* the sum of the *ee*-elementary diagrams whose external points belong to the same exchange loop, may substantially contribute to both S_τ and to the potential energy, if the potential has large exchange terms.

In evaluating $\langle H\rangle$, it is convenient to use the Jackson-Feenberg identity [17] for the kinetic energy, $\langle T\rangle$, with the result

$$\langle T\rangle = T_{JF} = T_\phi + T_F \quad , \tag{13}$$

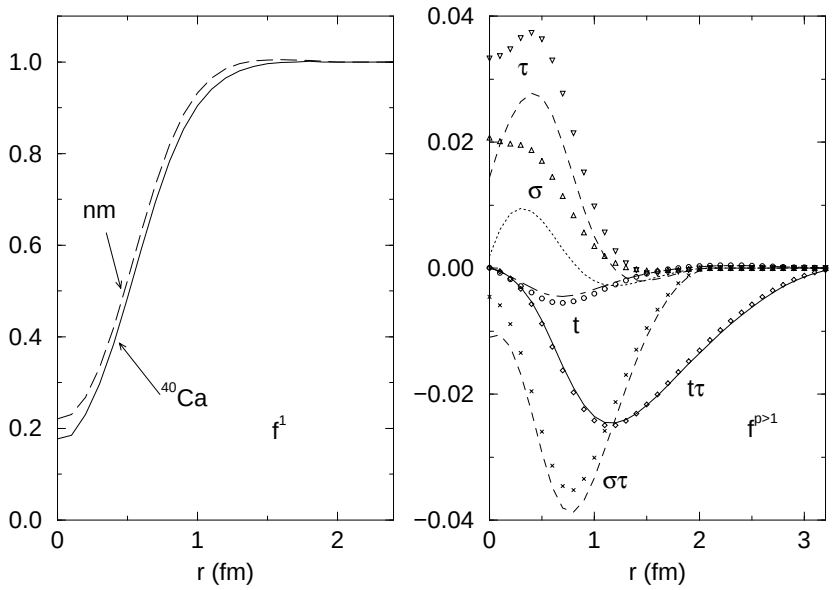

Figure 1. Correlation functions for ^{40}Ca and NM at saturation density. The operatorial correlations (right panel) are given as lines for ^{40}Ca and symbols for NM.

with

$$T_\phi = -A\frac{\hbar^2}{4m}\langle \Phi^* G^2 \nabla_1^2 \Phi - (\nabla_1 \Phi^*)\, G^2\, (\nabla_1 \Phi)\rangle \quad , \tag{14}$$

and

$$T_F = -A\frac{\hbar^2}{4m}\langle \Phi^* \left[G\nabla_1^2 G - \nabla_1 G \cdot \nabla_1 G \right] \Phi\rangle \quad , \tag{15}$$

where $G = \mathcal{S}\prod F_{ij}$. Ref.[12] describes how to compute T_ϕ in FHNC/SOC.

To evaluate T_F and the two-body potential energy $\langle v\rangle = V_2$, we define an interaction energy $W = T_F + V_2 = \langle H_{JF}\rangle$. The two-body operator, $H_{JF}^{ijk}(r_{12})$, is

$$H_{JF}^{ijk}(r_{12}) = -\frac{\hbar^2}{2m}\delta_{j1}\left\{ f^i(r_{12})\nabla^2 f^k(r_{12}) - \nabla f^i(r_{12})\cdot\nabla f^k(r_{12})\right\}$$
$$+ f^i(r_{12}) v^j(r_{12}) f^k(r_{12}) \quad . \tag{16}$$

In FHNC/SOC, W is split into four parts, $W = W_0 + W_s + W_c + W_{cs}$, where W_0 is the sum of the diagrams with only $p = 1$, central chains between the interacting points (IP), connected by H_{JF}; W_s sums diagrams having operatorial vertex corrections reaching the IP's and central chains; W_c contains diagrams with one SOC between the IP's; W_{cs} contains both. The lenghty formulas for W are again found in ref.[12].

3. ENERGETICS

The results presented in this section have been obtained with the single particle wave functions, $\phi_\alpha(i)$, generated by a harmonic oscillator well with parameter b.

Table 1

Breakup of the energy per nucleon, in MeV, for ^{16}O with the U6 potential. The J column gives the energies with the Jastrow corelated wave function, the O column those with the operatorial correlation and the CMC columns the cluster MonteCarlo results of ref.[18]. $E_{gs} = (\langle H \rangle - T_{cm})/A$.

	J	CMC(J)	O	CMC(O)
$\langle v^1 \rangle$	0.88	0.93(28)	2.33	2.35(43)
$\langle v^2 \rangle$	1.25	1.27(08)	1.97	2.00(13)
$\langle v^3 \rangle$			0.25	0.27(01)
$\langle v^4 \rangle$	2.40	2.43(12)	2.29	2.23(14)
$\langle v^5 \rangle$	-26.59	-26.24(26)	-32.03	-30.12(42)
$\langle v^6 \rangle$			-10.28	-9.77(09)
$\langle v \rangle$	-22.07	-21.56(25)	-35.47	-33.03(31)
$\langle T \rangle$	24.61	24.33(21)	31.16	29.45(33)
$\langle H \rangle$	2.54	2.77(09)	-4.33	-4.59(10)
E_{gs}	1.72		-5.15	

We kept b fixed ($b(^{16}O) = 1.543\ fm$ and $b(^{40}Ca) = 1.654\ fm$), even though it might be considered as a variational parameter. As far as the variational correlation, F_{ij}, is concerned, we follow ref.[9] and adopt an *Euler* correlation operator obtained by minimizing the energy at the second order of the cluster expansion, $\langle H_2 \rangle$. A corresponding choice was done in ref.[15] for NM. The variational parameters of the functions $f^p(r)$ are the *healing* distances, d_p, where $f^1(r \geq d_1) = 1$, $f^{p>1}(r \geq d_p) = 0$ and $(f^p)'(r = d_p) = 0$. As in NM, we use only two healing distances: d_c and d_t, for the central ($p = 1, 2, 4, 5$) and tensor ($p = 3, 6$) channels, respectively. An additional parameter is the quenching factor, α, of the $p > 1$ components of potential in the Euler equations. We have taken the U14 NM parameters, $d_c = 2.15\ fm$, $d_t = 3.43\ fm$ and $\alpha = 0.8$, on the assumption that the short range behavior of the correlation does not vary drastically in going from the infinite to the finite systems. It is clear that a more accurate variational search for each nucleus would provide a lower ground state energy.

The ^{40}Ca correlation functions are shown in Figure 1 and compared with the corresponding NM functions. They are similar, especially the longer ranged tensor parts. The most visible differences are found in the spin and isospin components and in the shortest range part of f^1.

The error in the S_1 sum rule, in FHNC/0, is well less than 1% in both nuclei

for either the Jastrow (J) or the operatorial (O) correlations. The same accuracy is found for S_2 and S_τ in the J-model after the insertion of the E_{ee}^{ex} diagram (FHNC-1). The situation worsens for the O-model, where FHNC/SOC violates the sum rules by a maximum amount of $\sim 9\%$, as it was already found in NM [15].

The U6 energetics is displayed in Table 1 for ^{16}O and Table 2 for ^{40}Ca, for the J and O correlations. The Tables provide the potential, kinetic and total energy per nucleon. The separated expectation values of the components of the potential are also shown, together with the ground state energy, E_{gs}, obtained by subtracting the center of mass kinetic energy, T_{cm}, from $\langle H \rangle$.

The ^{16}O results are compared with the CMC calculations of Pieper [18]. FHNC shows an error of $1-2\%$ for $\langle T \rangle$ and $\langle v_2 \rangle$ in the J case. The total energy error is larger ($\sim 9\%$) as $\langle H \rangle$ is given by the cancellation of two large numbers. The same situation is met in the O-model: the kinetic and potential energy errors are $5-7\%$. The absolute error in $\langle H \rangle$ is well less than 1 MeV, consistently with the estimated accuracy of FHNC/SOC in NM [15]. The OPE parts of the potential provide most of the binding since, in its absence, ^{16}O is not bound. The same holds in ^{40}Ca, where the introduction of tensor correlations and potentials increases the kinetic energy by ~ 5.6 MeV, compensated by an additional potential energy contribution of ~ -13.6 MeV, providing a bound nucleus.

In order to compare the theoretical energies with the experimental values one has to estimate the mean value of the full U14 interaction. Its $p > 6$ components represent the momentum dependent (MD) part of the potential, whose expectation value is more difficult to evaluate than U6 by means of cluster expansions. The usual strategy in NM is to include only low order (second and third) cluster MD contributions to $\langle v^{MD} \rangle$. This procedure is probably accurate for U14, since its MD part contributes to the g.s. energy by less than 1 MeV at $\rho_{NM} = 0.16$ fm^{-3} ($\Delta E_{NM}^{MD} = 0.44$ MeV), but it could be questionable for other potentials, as the recent Argonne v_{18} model [19]. Moreover, it is known that a pure two-body interaction does not reproduce the NM saturation (energy, density and incompressibility) and the binding energies of light nuclei, so three-nucleon interactions, v_{ijk}, are to be introduced. The TNI model of ref.[13] approximated the effect of v_{ijk} by adding two density dependent terms to U14: a repulsive TNR one, reducing the effect of the intermediate range part of v_{ij}, and an attractive TNA part. The TNR term was taken as

$$U14 + TNR = \sum_{p=1,14} [v_\pi^p(r_{ij}) + v_I^p(r_{ij})\ e^{-\gamma_1 \rho_{NM}} + v_S^p(r_{ij})] O_{ij}^p \quad , \tag{17}$$

where $v_{\pi,I,S}^p$ are the long-, intermediate- and short-range parts of the potential, ρ_{NM} is the NM density and $\gamma_1 = 0.15$ fm^{-3}. The TNA term was assumed to contribute as

$$TNA = 3\gamma_2 \rho_{NM}^2 e^{-\gamma_3 \rho_{NM}} \quad , \tag{18}$$

with $\gamma_2 = -700$ Mev fm^6 and $\gamma_3 = 13.6$ fm^3. The values of the γ-parameters were obtained by fitting the NM saturation properties in FHNC/SOC.

Here we evaluate the TNR contribution by using $[\rho_1(r_i)\rho_1(r_j)]^{1/2}$ in place of ρ_{NM} in (17) and

$$TNA = \frac{1}{A} \int d^3 r_1 \rho_1(r_1) \left[3\gamma_2 \rho_1^2(r_1) e^{-\gamma_3 \rho_1(r_1)} \right] \quad . \tag{19}$$

Table 2

As Table 1 for ^{40}Ca. The CMC results are not available in this case.

	J	O
$\langle v^1 \rangle$	-1.41	-0.21
$\langle v^2 \rangle$	1.57	2.30
$\langle v^3 \rangle$		0.29
$\langle v^4 \rangle$	2.99	2.71
$\langle v^5 \rangle$	-32.40	-39.48
$\langle v^6 \rangle$		-14.14
$\langle v \rangle$	-29.26	-47.28
$\langle T \rangle$	30.55	39.69
$\langle H \rangle$	1.30	-7.59
E_{gs}	1.01	-7.87

Table 3

Energies per nucleon (in MeV) for ^{16}O and ^{40}Ca with the U14+TNI interaction. See text.

	$\langle H \rangle_{U6}$	ΔE^{MD}	TNA	$\langle H \rangle_{U14+TNI}$	ΔE_c	E_{gs}	E_{gs}^{expt}
^{16}O	-1.88	0.33	-4.53	-6.08	0.05	-6.85	-7.72
^{40}Ca	-3.20	0.68	-4.59	-7.11	0.05	-7.35	-8.30

ΔE^{MD} is estimated in local density approximation (LDA) as

$$\Delta E^{MD} = \frac{1}{A} \int d^3 r_1 \rho_1(r_1) \Delta E_{NM}^{MD}[\rho_1(r_1)] \quad . \tag{20}$$

Table 3 gives the ^{16}O and ^{40}Ca energies with the U14+TNI interaction and the operatorial correlation model. ΔE_c is the Coulomb energy correction taken from ref.[11]. The experimental ground state binding energies per nucleon are underestimated by ~ 1 MeV in both nuclei. The MD contribution is enough low to makes us enduring the LDA in its evaluation. We are considerably satisfied with these results, most af all in consideration of the further energy lowering that could be obtained by a careful variational minimization and of the FHNC/SOC accuracy.

4. CONCLUSIONS

In this contribution we have presented some results for the ground state energy of doubly closed shell nuclei in *ls* coupling (^{16}O and ^{40}Ca) in the framework of the correlated basis function theory. The correlated wave function includes central and tensor correlations, whose non commutativity does not allow for a complete FHNC treatement, contrary to the purely scalar case. We have extended the single operator chain approximation scheme (as used in realistic studies of nuclear and neutron matter) to the finite nuclei. The U6 truncation of the realistic Urbana v_{14} nucleon-nucleon potential has been adopted as a test.

By the analysis of the sum rules we have shown that FHNC/SOC provides an accurate one-body density. A comparably good accuracy is obtained for the normalizations of the two-body density (S_2 and S_τ) when tensor correlations are not included. Their insertion slightly worsens the excellent fullfiment of $S_{2,\tau}$, but the maximum violation is ~ 9 %, similar to what was found in nuclear matter.

The comparison of the energy contributions in ^{16}O for the U6 interaction with the cluster Monte Carlo results shows a maximum disagreement varying from ~ 2 % for the Jastrow model to ~ 7 % for the tensor model. The absolute error in the ground state energy per nucleon is well less 1 MeV, compatible with the estimated accuracy of the FHNC/SOC approach in nuclear matter at saturation density.

The ground state expectation value of the complete realistic U14+TNI interaction has been evaluated by estimating the small momentum dependent contribution in local density approximation. The binding energies are about 1 Mev lower than the experimental values. Further improvements are reasonably to be expected by a better variational minimization. To our knowledge and opininion, this is one of the very few reliable microscopic evaluations of the g.s. energy of these nuclei with a realistic hamiltonian. Recently derived nuclear potentials provide a higher quality fit to the nucleon-nucleon scattering data, however their momentum dependence is stronger than in U14. Consequently, a better than LDA treatment of this part is imperative if they are to be used in the nuclei we have studied. Our group is working along this line, as well as to the insertion of explicit three-nucleon forces.

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